Monte-Carlo calculation of longitudinal and transverse resistivities in a model Type-II superconductor

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We study the effect of a transport current on the vortex-line lattice in isotropic type-II superconductors in the presence of strong thermal fluctuations by means of 'driven-diffusion' Monte Carlo simulations of a discretized London theory with finite magnetic penetration depth. We calculate the current-voltage (I-V) characteristics for various temperatures, for transverse as well as longitudinal currents I. From these characteristics, we estimate the linear resistivities $R_{xx} = R_{yy}$ and R_{zz} and compare these with equilibrium results for the vortex-lattice structure factor and the helicity moduli. From this comparison a consistent picture arises, in which the melting of the flux-line lattice occurs in two stages for the system size considered. In the first stage of the melting, at a temperature T_m, the structure factor drops to zero and R_{xx} becomes finite. For a higher temperature T_z, the second stage takes place, in which the longitudinal superconducting coherence is lost, and R_{zz} becomes finite as well. We compare our results with related recent numerical work and experiments on cuprate superconductors.

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I. INTRODUCTION

The statistical mechanics of vortex lines in type-II superconductors has been the subject of intense study after the discovery of the high-temperature superconductors. Due to the large thermal fluctuations and pronounced anisotropies of these materials, thermal wandering of vortex lines leads to a rich phase diagram [1,2]. Numerous experiments [3–7] and computer simulations [8–21] were interpreted as evidence for the scenario of a vortex-lattice melting transition into a vortex-liquid phase. Most convincing evidence for the existence of a first-order phase transition separating the vortex lattice from a liquid phase comes from a recent calorimetric measurement of the specific heat in YBCO [6] and from magnetization measurements in YBCO [4] as well as BiSCCO [5]. An explanation of the magnitude and temperature dependence of the observed characteristic entropy and magnetization jumps has been given in a recent work by Dodgson *et al.* [22].

One interesting aspect of the melting transition is the question of whether it coincides with a complete loss of c-axis correlation (i.e. decoupling of the vortex lines into independent 'pancakes' in the Cu-O layers). A recent transport measurement on untwinned YBCO by Righi *et al.* [23] indicates that just above the melting temperature, the vortices are still correlated over a few microns, and become fully decoupled only at a distinctly higher temperature.

On the theoretical side, the properties of the vortex liquid phase have been intensively studied. Some time ago Li and Teitel [11] numerically studied the (uniformly frustrated) 3D XY model on a cubic lattice, and found a melting transition into a liquid with longitudinal superconducting coherence. The longitudinal superconductivity, signalling a c-axis vortex correlation over the full system thickness, was found to be lost at a distinct temperature above the melting temperature. In later work including screening effects using the lattice London Model, a similar two-stage melting transition was found by Chen and Teitel [12,14]. Recently, a two-stage transition was also found by Ryu and Stroud [18] using a 3D XY model on a stacked triangular lattice, for a frustration lower than studied in earlier work by Hetzel *et al.* [9]. When the intermediate liquid with longitudinal coherence would persist into the thermodynamic limit (very large system thickness), it would be the realization of the so-called line-liquid phase proposed in Ref. [24].

In this paper we study the dynamical properties of the lattice London model and compare them with the behavior of equilibrium quantities as studied in Refs. [12,14,16,25].

II. LATTICE LONDON MODEL AND MONTE CARLO METHOD

The Hamiltonian of the isotropic lattice London model, at constant induction B, reads:

$$\mathcal{H} = 4\pi^2 J \sum_{i,j,\mu} q_\mu(\boldsymbol{R}_i) q_\mu(\boldsymbol{R}_j) g(\boldsymbol{R}_i - \boldsymbol{R}_j) \quad (1)$$

where $J = \Phi_0^2 d/(32\pi^3\lambda^2)$ (with λ the magnetic penetration depth) and $g(\boldsymbol{R})$ is the London interaction with Fourier components

$$g(\boldsymbol{k}) = \frac{1}{\kappa^2 + (d/\lambda)^2} \quad (2)$$

and $\kappa^2 = \sum_\mu \kappa_\mu^2$ with $\kappa_\mu^2 = 2 - 2\cos k_\mu$ ($k_\mu = 2\pi n_\mu / L_\mu$, $n_\mu = 0, 1, ..., L_\mu - 1$). Here we assumed an $L_x \times L_y \times L_z$ lattice with periodic boundary conditions. At every dual lattice site $\boldsymbol{R}$ of our square lattice, the integer variable $q_\mu(\boldsymbol{R})$ denotes the vorticity or number of flux-line unit elements in the direction $\mu = x, y, z$. The $q_\mu(\boldsymbol{R}_i)$ are subject to the continuity constraint $\sum_{\boldsymbol{e}_\mu} [q_\mu(\boldsymbol{R}_i) - q_\mu(\boldsymbol{R}_i - \boldsymbol{e}_\mu)] = 0$. Here $\boldsymbol{R}_i - \boldsymbol{e}_\mu$ runs over nearest neighbor sites of $\boldsymbol{R}_i$. λ is the magnetic penetration depth and d the lattice constant. The Hamiltonian (1) can be derived from the discrete version of the London free energy [10,14,33].

Monte Carlo sampling of the phase space for the variables $q_\mu(\boldsymbol{R})$ at constant B is performed as follows. In the simulations, the initial configuration is prepared to contain the number of vortex lines corresponding to the value chosen for B. A Monte Carlo update step consists of adding at a given site a closed $d \times d$ square loop of unit vorticity with an orientation chosen randomly from the six possible ones. This scheme preserves the magnetic induction B with components $B_\mu = \frac{\Phi_0}{d^2\mathcal{V}} \sum_j \langle q_\mu(\boldsymbol{R}_j) \rangle$. ($\mathcal{V} = L_x L_y L_z$). The standard Metropolis algorithm is employed to accept or reject the new configuration. For equilibrium calculations, one uses (1) to calculate the energy change ΔE between the old and the new configuration. To simulate the presence of a uniform transport current $\boldsymbol{j}$, we introduce an additional bias in the acceptance rates by subtracting or adding $(\Delta E)_j = \Phi_0 \mid \boldsymbol{j} \mid d^2/c$ to the energy change ΔE when an elementary loop is added whose normal vector is pointing in the same direction as $\boldsymbol{j}$ or $-\boldsymbol{j}$ respectively. We measure the magnitude of the current in terms of the dimensionless quantity $\boldsymbol{\alpha} \equiv \boldsymbol{j}\Phi_0 d^2/(Jc)$. The dimensionless voltage V_μ is obtained by measuring the rate at which vortex jumps in the μ direction are occurring. This 'driven-diffusion' method was used before in Refs. [26].

III. RESULTS

Our calculations are carried out on a $15 \times 15 \times 15$ cubic lattice, with a magnetic field running in the z direction. We choose the filling fraction $f = 1/15$ and $\lambda = 5d$, as in Refs. [12,14]. Runs were taken consisting of 16,384 (high currents) up to 262,144 (low currents) Monte Carlo sweeps through the lattice, half of which were used for equilibration.

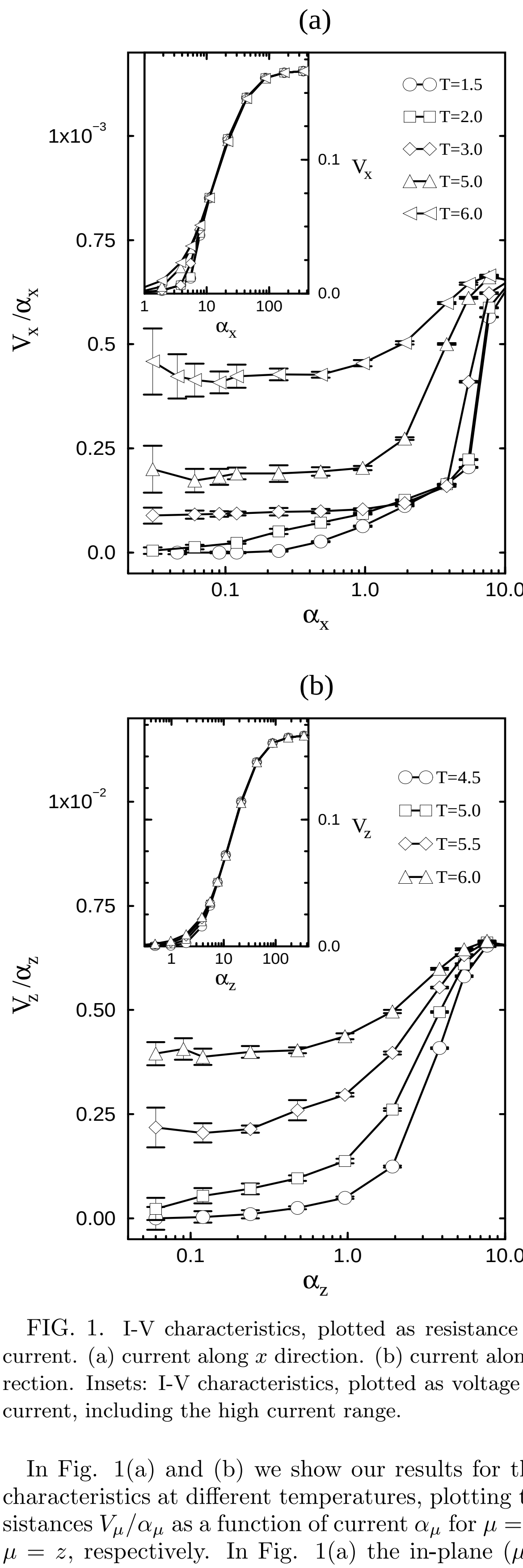

FIG. 1. I-V characteristics, plotted as resistance versus current. (a) current along x direction. (b) current along z direction. Insets: I-V characteristics, plotted as voltage versus current, including the high current range.

In Fig. 1(a) and (b) we show our results for the I-V characteristics at different temperatures, plotting the resistances V_μ/α_μ as a function of current α_μ for $\mu = x$ and $\mu = z$, respectively. In Fig. 1(a) the in-plane ($\mu = x$) resistance is shown. For the lowest T shown ($T = 1.5$

in units of J/k_B), the resistivity drops to zero below a finite current value (critical current), and thus the linear resistivity

$$R_{xx} \equiv \lim_{\alpha_x \to 0} \frac{V_x}{\alpha_x} \tag{3}$$

is zero. For $T = 2.0$ no clear critical current is observed, but again we estimate R_{xx} to be zero (or very small). For the higher T's studied, we find that the I-V characteristic is linear (constant resistance) for sufficiently small currents. For high currents, the I-V characteristics become independent of temperature (see insets in Figs. 1(a) and (b)). In the high-current limit the voltage saturates at the value 1/6, corresponding to acceptance of all the Monte Carlo trial moves in the direction of the Lorentz force.

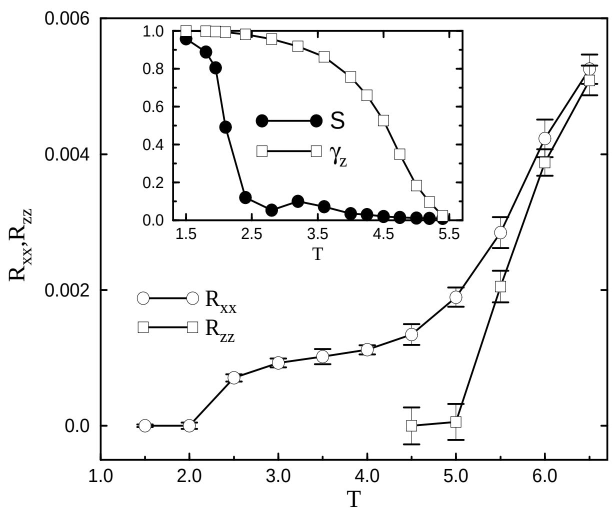

FIG. 2. Linear resistivities vs. T. Circles: in-plane. Squares: out-of-plane. Inset: temperature dependence of the vortex-lattice structure factor $S \equiv S(\boldsymbol{k}_s)$, with k_s the smallest reciprocal lattice vector of the ground state vortex lattice, and the helicity modulus γ_z, calculated at $\boldsymbol{j} = 0$.

In Fig. 2 we plot the linear resistivities R_{xx} and R_{zz} (estimated from the I-V characteristics of which representative ones are shown in Fig. 1) as a function of T. We distinguish three temperature regions with different dissipative properties. For low T, both R_{xx} and R_{zz} are zero. This is the flux-line lattice state, stabilized against small currents by the artificial pinning effect of the discrete mesh in our simulation. For intermediate T, R_{xx} becomes finite but R_{zz} is still zero. Finally, for high T, both transport coefficients become nonzero. For comparison, we include equilibrium (i.e. $\boldsymbol{j} = 0$) results for the structure factor S and the helicity modulus γ_z in the inset of Fig. 2. These equilibrium results were obtained before in Refs. [12,14]. The temperature at which the in-plane linear resistance becomes nonzero coincides with the melting temperature T_m of the flux-line lattice as found from the decay of the equilibrium structure factor [28]. Furthermore, the temperature at which the out-of-plane linear resistance R_{zz} becomes nonzero coincides with the temperature T_z at which the $\boldsymbol{j} = 0$ helicity modulus γ_z vanishes (see inset). Here γ_z was calculated as explained in detail in Ref. [25]. This is consistent with the interpretation of γ_z as a measure of longitudinal superconducting coherence or longitudinal superconductivity. Thus our transport calculations confirm the two-stage melting picture found in equilibrium simulations of this model [12,14], in which there is an intermediate vortex-liquid regime with superconductivity along the vortex lines. In this intermediate regime $T_m < T < T_z$ the vortex lines are c-axis correlated over the full system thickness $L_z = 15$ simulated. For $T > T_z$ the longitudinal correlation length becomes smaller than L_z. At some even higher T_d (decoupling temperature), the c-axis correlation should be lost completely.

IV. DISCUSSION

As our results are obtained for a finite system size, it is not clear from them whether the two-stage melting scenario persists into the thermodynamic limit. In fact, we believe that this will not be the case. In Refs. [12,14] it was found that the T_z decreased with increasing system thickness L_z. In Ref. [19], the L_z dependence of T_z was studied for the uniformly frustrated Villain Model. There it was also found that the intermediate temperature region decreased in size with increasing L_z. We interpret this finite-size behavior as a manifestation of a c-axis correlation length that, in a thick system, is finite and large just above the melting temperature and shrinks with increasing temperature until a decoupling temperature T_d is reached. Thus, what these simulation results *do* predict for real (i.e. thick) systems is that the vortex lattice melts into a liquid in which the vortex lines are c-axis correlated over many layer distances, i.e. far from decoupled. Only for higher temperatures a crossover takes place into a decoupled regime above T_d. This scenario agrees well with the transport experiments on YBCO by Righi *et al.* [23], that indicate that just above the melting temperature, the vortices are still correlated over a few microns [27], i.e. thousands of Cu-O layer distances, and become fully decoupled only at a distinctly higher temperature. In contrast, measurements on BiSCCO by Doyle *et al.* [7] were interpreted as evidence for a simultaneous melting and decoupling. This is consistent with recent Monte-Carlo simulations of a strongly anisotropic modified 3D XY model by Koshelev [20], in which it was found that the longitudinal helicity modulus drops to zero close to the melting temperature already for $L_z = 40$ and larger. We note that such a behavior was also found for $L_z = 40$ in a recent Monte Carlo study of an only slightly anisotropic 3D XY model, in which the melting

transition was investigated upon cooling [21].

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